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13. ABSTRACT (Maximum 200 words) Algorithms, simulations and modeling for fluid mixing and complex flow were developed. Our front tracking algorithm was improved for its accuracy and conservation properties. Local mesh refinement was added. Simulations in agreement with experiment were obtained. New models of the fluid mixing process were derived, which were also compared to experimental data.			
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A REPORT OUTLINE

1. ARO PROPOSAL NUMBER: 42254-MA
2. PERIOD COVERED BY REPORT: 15 June 2001 – 14 June 2004
3. TITLE OF PROPOSAL: Multiscale Modeling of Complex Physics: Fluids, Solids, Optics
4. CONTRACT OR GRANT NUMBER: DAAD19-01-1-0642
5. NAME OF INSTITUTION: State University of New York at Stony Brook
6. AUTHOR OF REPORT: James Glimm
7. APPENDICES, ILLUSTRATIONS, and TABLES: None
8. PROBLEM SOLVED:
 - Improved Front Tracking algorithms: Fully conservative, higher order accurate, automatic mesh refinement (AMR) and locally grid based resolution of interface bifurcations (for improved accuracy and robustness)
 - Simulations and theory for turbulent mixing rates in agreement with experimental data.

- Models for solution error for numerical simulation were developed and applied to engineering problems.
- Parallel FDTD photonics code with totally absorbing boundary conditions
- New algorithms for structural biology on ultra-fast parallel computers
- Technology Transfer to National Laboratories

9. SUMMARY OF MOST IMPORTANT RESULTS: See below.

10. TECHNOLOGY TRANSFER: Our photonics work is conducted as a collaboration with C. Bowden and M. Scalora of Redstone Arsenal. We interact with Tim Wright of ARL. J. Glimm has been chair of the External Advisory Board of the Weapons and Materials Science Directorate of ARL and a member of the Technical Advisory Board of ARL. He was also a member of the External Review Committee for the Dynamical Experimentation Division of Los Alamos National Laboratory.

The simulation code FronTier is in use at Los Alamos National Laboratory, both for fluid and for solid deformation modeling. It is used in fluid modeling in collaboration with staff of Livermore National Laboratory, Sandia National Laboratory and Brookhaven National Laboratory.

Work on photonics is in use for engineering design studies at Brookhaven National Laboratory.

Work on structural biology is in collaboration with crystallographers at Brookhaven National Laboratory.

Work on uncertainty quantification is in use at Los Alamos National Laboratory.

11. SCIENTIFIC PERSONNEL SUPPORTED BY THIS PROJECT AND DEGREES AWARDED WHILE EMPLOYED ON PROJECT:

- (a) Senior Personnel: Bradley Plohr
- (b) Post Docs: Yingjie Liu, Hyeonseong Jin, Erwin George
- (c) Graduate Students: Erwin George, Wei Guo, Jason Heller, Xinfeng Liu, Tianshi Lu, Jee-Yeon Nam, Shiqiang Wang, Yan Yu, Ming Zhao
- (d) Ph. D. Degrees Awarded (Students Supported by this Grant): Erwin George, Wei Guo, Jee-Yeon Nam

12. REPORT OF INVENTIONS (BY TITLE ONLY): No inventions were produced by the researchers.

13. COPIES OF TECHNICAL REPORTS: Sent Previously

B LIST OF MANUSCRIPTS SUBMITTED OR PUBLISHED UNDER ARO SPONSORSHIP DURING THIS REPORTING PERIOD, INCLUDING JOURNAL REFERENCES

B.1 Peer Reviewed Publications

- [1] S. I. Abarzhi, J. Glimm, and An-Der Lin. Rayleigh-Taylor instability for fluids with a finite density contrast. *Phys. Fluids*, 15:2190–2197, 2003.
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C SUMMARY OF MOST IMPORTANT RESULTS

Introduction. The principal thrust of our new simulations were fluid interface instabilities, solid dynamics, uncertainty quantification, structural biology and photonics. All of this work has joined developments in theory and modeling to our simulation results.

Additional Army-related activities of the project PI, James Glimm, within this reporting period include: chair of the External Advisory Board for the Weapons and Material Science Directorate of the ARL; a member of the Technical Advisory Board of ARL; member of the Technical Advisory Board of the Dynamic Testing Division of Los Alamos National Laboratory; and scientific interaction with Tim Wright of ARL and Chuck Bowden and Michale Scalora of Redstone Arsenal.

Improved Front Tracking Algorithms Four important improvements have been added to our Front Tracking simulations. These are:

- A capability for MHD has been added, with sharp boundaries between distinct MHD fluids having distinct conductivities.
- Automatic Mesh Refinement (AMR) has been added, through merger of our FronTier code with the LLNL Overture code. The AMR is patch based, and follows the Berger-Colella algorithm.
- Robust simple interface bifurcations have been achieved in 3D through use of a locally grid based interface description algorithm. Regions containing bifurcations have been reconstructed based on a reduced, grid related interface description. The algorithm is very robust. See [20, 47].
- Fully conservative front propagation has been achieved through a new tracking algorithm which tracks a discontinuity surface in space and time, [40, 39, 38, 41].

Simulations and Theory for Turbulent Mixing Definitive results have been obtained for the simulation [6, 26, 21, 15] of Rayleigh-Taylor flows, with the first agreement of simulation with experiment and theory [9, 5] for three dimensional acceleration driven (Rayleigh-Taylor) turbulent mixing. The importance of the agreement obtained by the FronTier simulations with experiment and theory is emphasized by the disagreement, by a factor of about two, between most codes and experiment for this problem. Instabilities in axisymmetric implosions and explosions were simulated [27, 28]. Validation studies and an exploration of the influence of axisymmetry in the problem definition on the statistics of the chaotic mixing were performed. Agreement with laser driven experiments [13] was obtained.

Elastic-Plastic Flow. Validation studies for the Front Tracking code FronTier-Solid have been performed [52]. Front Tracking is advantageous relative to traditional Langrangian codes because the fixed Eulerian computational mesh is not subject to mesh distortion; it is advantageous relative to standard Eulerian codes because the tracking eliminates spurious numerical diffusion at interfaces and the need for artificial mixed-material computational cells. FronTier-Solid is a two-dimensional solid dynamics code based on a fully conservative formulation of the governing equations for large-strain deformation, a hyperelastic equation of state that allows for large volumetric change, and a rate-dependent plasticity model for

high strain rates. The code features conservative finite differencing, a Riemann solver that accounts for the nonlinearity of longitudinal waves, and an implicit method for integrating the plastic source term.

The Richtmyer-Meshkov shock driven instability was studied in elastic materials (i.e. with strength) in a Stony Brook Ph.D thesis [48]. The work focused on linearized solutions; it serves as a validation standard for nonlinear simulations. The unperturbed solution is obtained using the Riemann solver that is part of the FronTier Solid code. The corresponding linearized equations are solved numerically. The main result is a prediction of the growth rate of the perturbation amplitude.

Uncertainty Quantification. The purpose of this project is to assess and quantify the uncertainty of predictions made with simulation codes. As the codes are being used to make operational decisions, and as the degree of experimental testing is diminished, the verification and validation (V&V) of simulation codes becomes of increasing importance. Quantification of uncertainty may be viewed as an extension of whole V&V effort. It goes beyond asking the question, is the simulation correct, and more quantitatively, it asks, ‘how correct is the simulation?’, with a quantitative answer expressed in the form of error bars, confidence intervals, or some measure of uncertainty. In our earlier papers we found that the interplay between the forward and inverse problems, with Bayesian analysis to include the added information of experiments, was important. Also the study of probabilistic error models for numerical solution errors is important. Following this lead, we have begun a probabilistic study of solution errors [30, 31, 12], based on computer experiments to generate the numerical errors.

The point of view we have developed appears to be rather original, as we are not aware of comparable studies of numerical solution error. Most prior work on solution error assumed that the simulation is already fully resolved, and that the numerical solution is within the range of asymptotic convergence, so that theory based on numerical estimates of order of convergence can be applied. All of these assumptions are not likely to be valid for the simulation of complex problems.

Photonics. This is a new project, conducted in collaboration with C. Bowden and M. Scalora of Redstone Arsenal and their collaborators. We have developed a parallelized FDTD code with nonreflecting boundaries to allow simulations in complex 3D geometries for photonic crystals and other photonic devices [51]. We have built on our prior experience in parallel software development, and in construction of low cost parallel hardware.

Our program is specially designed to study finite photonic devices with three-dimensionally heterogeneous dielectrics. The changes in the dielectric function occur on the scale of the electromagnetic wavelength and the contrast between the dielectric constants is large. We consider applications to finite devices for frequency doublers and high quality cavities for VCSEL lasers. The code is being used to simulate application specific device geometries to resolve design issues. We are working with experimental groups to model the devices and optimize the parameter values.

We have conducted design studies for RF cavities and other accelerator components at Brookhaven National Laboratory using this code.

Structural Biology on High Performance Hardware We investigated [11, 10] the use of novel high performance hardware for structural biology (MD and MC) simulations.

The hardware target was a special purpose design, QCDOC, primarily intended for quantum gauge theory calculations. This machine is a precursor to the general purpose IBM machine BG/L, and both are unique in using a mesh rather than a switch for parallel communication. As a result, the machine has very attractive price performance behavior for large size (30K to 150K processor) configurations. We developed a simulation model of the force field calculation (especially for the Coulomb force), and project that it will be possible to simulate 100K atoms in an all atom simulation for up to 1 to 10 μ sec. We are developing an MD simulation code to run on QCDOC and in the meantime we are simulating Bolulinum, as a target molecule. This work is conducted in collaboration with crystallographers at Brookhaven National Laboratory.

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